

File Types

Molviewer currently reads 3 file types. I will happily add any additional formats that I receive specifications for.

PDB files - These files are expected to have .ent extensions. This is the Brookhaven Protein Database file format. I haven't tested it very thoroughly, but it should work for most files. "CONNECT" records are used to determine bonding, so line drawings may be incomplete if this file format is read (see future plans). More information on this format can be found via anonymous ftp to [pdb.pdb.bnl.gov](ftp.pdb.bnl.gov).

Only the first entry from a PDB file is used. The program will stop reading atoms when it hits a TER record.

MV files - THIS FORMAT IS CURRENTLY IN TRANSITION. I RECOMMEND NOT USING IT FOR NOW.

This is my own file format for use with a variety of programs I use in the lab. Each molecule is stored as 2 files. One contains a list of atoms and coordinates, the other contains bond information. The file with atomic coordinates has a .crd extension. When opening a file pair, this is the file to open. It's format is:

```
# <optional comments>  
<seq #> _<atom> _<x> _<y> _<z>
```

<seq #> is the number to use for this atom in the bond file. It MUST start with 0 and increase by 1 each atom.

_ represents whitespace, I use tabs, but spaces are ok too.
<atom> is the 1 or 2 letter symbol for the atom. It must be capitalized.

<x>, <y>, <z> are self-explanatory.

The bond file has the .bnd extension. If it isn't present the molecule will still be read, but can only be viewed with the

space-filling model. It's format is:

<bond type><atom 1>_<atom 2>_<length>_<weight>

<bond type> is a single character. For this program it should always be "L".

<atom 1> and <atom 2> are the sequence numbers of the connected atoms in the .crd file.

<length> and <weight> aren't used in this program and may be omitted.

Alchemy files - This is the file format used by the popular chemistry program for the IBM and MAC. The format is pretty self-explanatory. Several example files are included. This is the only format for which saving is currently supported.